

EDUCATION

BE Computer Science , Birla Institute of Technology and Science, Pilani – Goa Campus	2020-2025(expected)
MSc Chemistry , Birla Institute of Technology and Science, Pilani – Goa Campus	2020-2025(expected)

SKILLS

Tools and Languages	Python, Git, LaTeX, C, MySQL, PyTorch, TensorFlow, Pandas, CI/CD Pipelines, AWS, Azure
Quantitative Research	Machine Learning, Drug Discovery, Generative AI, NLP, LLMs

TECHNICAL EXPERIENCE

Visiting Researcher Intern Yale University	Jun 2024 — Present New Haven, NY
<ul style="list-style-type: none">Conducting research on molecule generation models using geometric deep learning with Prof. Smita KrishnaswamyDeveloping novel algorithms to enhance molecular design efficiency	
Research Intern Harvard Medical School	Dec 2023 — Present Remote
<ul style="list-style-type: none">Investigating the neural mechanisms of language processing using AI models under Prof Gabriel KreimanApplying advanced machine learning techniques to analyze neural data, contributing to a deeper understanding of language cognition	
Research Fellow Deep Forest Sciences	Jun 2023 — Present Remote
<ul style="list-style-type: none">Developed tools for AI-aided retrosynthesis, molecule & materials discoveryBuilt infrastructure to train Molecular LLMsSemifinalist at the Standard Industries Chemical Innovation Challenge, awarded prize money of \$10,000Migrated models in the open-source drug discovery toolkit DeepChem from TensorFlow to PyTorch, increasing user base by 92%	
Product Engineering Intern Sprinklr	Jun 2024 — July 2024 Gurgaon, India
<ul style="list-style-type: none">Developed an ASR transcription evaluation pipeline using NLP techniquesCreated a custom scoring metric for evaluating transcripts in production, enhancing accuracyImproved productivity of product managers by 2x through streamlined evaluation processes	
Student Researcher APPCAIR, Birla Institute of Technology & Science, Pilani	2022 — Present Goa
<ul style="list-style-type: none">Researched the use of Large Language Models to generate novel molecules for drug discovery and predict their synthesizabilityDevised deep learning methods to predict protein residue binding sitesEvaluated BERT and Transformer-based architectures for protein residue binding location prediction	
Research Intern Amrita Vishwa Vidyapeetham	2021 — 2023 Bangalore, Karnataka
<ul style="list-style-type: none">Published a paper titled "Speech to Equation Conversion using a PoE Tagger"Designed a novel NLP architecture to handle variability in spoken mathematical equations	
Data Science Intern Skan.ai	Jun 2022 — Aug 2022 Bangalore, Karnataka
<ul style="list-style-type: none">Implemented data anonymization techniques using machine learning for process mining applicationsDeveloped an AI/ML pipeline for real-time data anonymization, improving processing speed by 30%	
Research Intern Pixis.ai	Feb 2022 — May 2022 Bangalore, Karnataka
<ul style="list-style-type: none">Optimised Algorithmic Trading App to identify arbitrage opportunities to do a round trip trading with different currencies from 30 min to 2 sec	

PUBLICATIONS

- V. Shreyas**, J. Siguenza, K. Bania & B. Ramsundar "Open Source Molecular Processing Pipeline for Generating Molecules" *Molecular Machine Learning Conference (MoML)* 2024
- V. Sathyanarayana and **V. Shreyas** "Prompting with Justification and Confidence: Extracting Information and Relationship using LLMs" (Under Review)
- V. Shreyas** and A. Swati, "Predicting ATP binding sites in protein sequences using Deep Learning and Natural Language Processing" *3rd Annual AAAI Workshop on AI to Accelerate Science and Engineering (AI2ASE)*, 2024.
- Mestha, H., Agrawal, T., Bania, K., **V. Shreyas** & Bhisikar, Y. (2024). "CountCLIP-[Re] Teaching CLIP to Count to Ten". *arXiv preprint arXiv:2406.03586*.
- P. Basa Pati and **V. Shreyas**, "Speech to Equation Conversion using a PoE Tagger," *2022 IEEE 7th International conference for Convergence in Technology (I2CT)*, 2022, pp. 1-4, doi: 10.1109/I2CT54291.2022.9824252.

PROJECTS

Metamorph - Generative AI **May 2023 — July 2023**
Building an **emotionally responsive Humanoid** bot with **knowledge capture** , **speech text generation** using Generative Large Language Models

ACTIVITIES

ML Lead, Google Developer Student Clubs, BITS Goa **2022 — 2023**

- Guided a group of 25+ ML enthusiasts , conducted weekly ML training sessions
- Organized hackathons , mentored in ML model building , and fostered exploration in ML research.

Sub-Coordinator, Sruttilaya, BITS Goa **2022 — 2023**

- Awarded Certificate of Recognition by the Chief Minister of Goa for Performing a cultural show in the QS India Summit 2023, held in Goa.
- Organized various classical concerts and Led a team of 25+ to bring in Indian Oil and First Edition Arts as sponsors for the event Sursangam which had a footfall of 500 people and 300 Live-stream attendees . Increased revenue of the club by 100

AWARDS AND RECOGNITIONS

2nd Runner up | *ACM Goa Chapter's event PitchIt!* *Apr 2024*
Best Logical Thinker | *Sri Kumarans Childrens Home CBSE* *Feb 2020*
Silver Standard | *The Duke of Edinburgh's International Award* *Aug 2018*
Runner Up | *Vidyarthi Vigyan Manthan* *May 2018*
1 out of 50 students chosen to participate in National Camp, Ranked **2nd out of 50 students** in the south Zone at National Camp

CERTIFICATIONS

Machine Learning *Stanford University, Coursera. May 2022*
Neural Networks and Deep Learning *DeepLearning.ai, Coursera. May 2022*
Natural Language Processing with Deep Learning *Stanford University. May 2022*
Fundamentals of Accelerated Data Science with RAPIDS *Nvidia DLI. Issued July 2021* [Certificate](#)
Python 3 Programming Specialization *University of Michigan, Coursera. December 2020*
Introduction to Artificial Intelligence (AI) *IBM, Coursera. Issued November 2020* [Certificate](#)
What is Data Science? *IBM, Coursera. Issued October 2020* [Certificate](#)